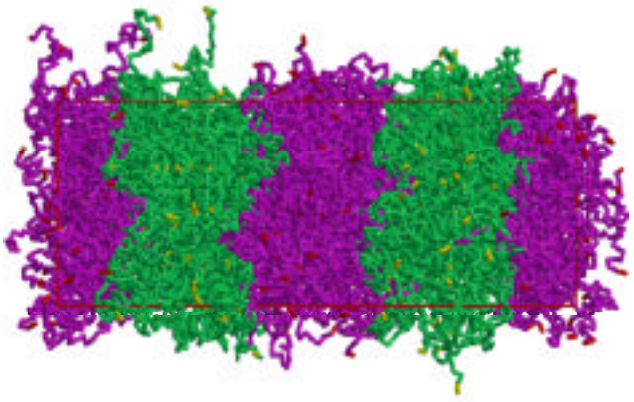
VI.F Interfacial Behavior of Symmetric Diblock Copolymers

Introduction: Polymers are one of the 20th century miracle materials. Light weight, high strength, ease of formability, and other desirable properties have led to a vast array of new and improved products. Polymer systems are notably complex materials in which both the local chemical interactions and the conformations of the polymer chains play important roles in determining properties. The range of characteristic length and time scales span many decades. The properties and phenomena exhibited by a single chain in a dilute solution are markedly different from an entangled polymer melt or a cross-linked network. Increasingly, computer simulations are playing an important role in testing the basic assumptions of theoretical models and interpreting experimental results. Studies of phase transformations provide an illustrative example.

Calculational Notes: The calculations involve molecular dynamics simulations of polymer melts and networks of 50,000 to 1,000,000 monomers and up to 200 million time steps. The classical interaction potentials are either explicit or united atom for short chains and coarse- grained bead-spring models for long chains. The calculations run on systems from workstations to both shared memory and distributed memory clusters.



Lamellar phanse in a symmetric diblock copolymer system

Results: The figure shows a snapshot of a diblock copolymer system in the ordered lamellar phase. The two incompatible halves of each chain are jointed at one point. To determine the dynamic properties, it is necessary to simulate for very long times to properly allow for diffusion of the chains parallel and perpendicular to the interface. For temperatures above the order-disorder transition, the polymers form a disordered phase. However at low temperatures, various complex ordered phases form. The nature of the ordered phase depends on the relative amounts of the two components. In the symmetric case, shown here, the ordered phase is lamellar. The yellow and dark red indicate the ends of the chain. As the temperature increases the interface between the two phases becomes more disordered.

Significance: The ability to model a variety of homopolymer systems, from melts to cross linked networks or rubbers, has led to new insight into the mechanisms that control the complex dynamical and relaxation processes. As computational power has increased over the past few years, there has been rapid progress in bringing new insights to a number of important technological issues, including how to strengthen the interface between incompatible polymers. The simulations are able to provide essential features of the phase diagram of immiscible polymer blends. New terascale computers provide the opportunity to build accurate models of polymers at interfaces. More accurate models are a necessary prerequisite to a better understanding of complicated phenomena such as adhesion and failure and to a study of polymers under shear, which is a critical element in the technological process of polymer extrusion.